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The Effect of Variable Composition Equilibrium Thermochemistry in Constant Breech Pressure (CBP) Gun Simulations

by Anthony J. Kotlar

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Anthony J. Kotlar
Weapons and Materials Research Directorate, ARL

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14. ABSTRACT

The limiting case of the constant breech pressure (CBP) gun is often invoked to predict the maximum velocity or efficiency of a gun system. Typically this calculation is done using a Lagrange pressure gradient and by considering the chamber composition to be chemically inert. In this study, CBP gun calculations are performed with full equilibrium chemistry obtaining throughout the ballistic cycle. The three well-defined thermodynamic states that completely characterize the energetics of this gun system are identified. This method represents an "exact" calculation of the optimized CBP (before burnout), Lagrange pressure gradient, no-loss gun system. A comparison of predicted-to-measured muzzle velocities is made for a number of fielded and experimental guns, and several hypothetical systems are examined. The comparison of calculated muzzle velocities permits an assessment to be made of the importance of chemical reactivity throughout the ballistic cycle.

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THE EFFECT OF VARIABLE COMPOSITION EQUILIBRIUM THERMOCHEMISTRY IN CONSTANT BREECH PRESSURE (CBP) GUN SIMULATIONS

Anthony J. Kotlar

U. S. Army Research Laboratory, Aberdeen Proving Ground, MD, 21005-5066, USA.

The limiting case of the constant breech pressure (CBP) gun is often invoked to predict the maximum velocity or efficiency of a gun system. Typically this calculation is done using a Lagrange pressure gradient and by considering the chamber composition to be chemically inert. In this study, constant breech pressure gun calculations are performed with full equilibrium chemistry obtaining throughout the ballistic cycle. The three well-defined thermodynamic states that completely characterize the energetics of this gun system are identified. This method represents an "exact" calculation of the optimized constant breech pressure (before burnout), Lagrange pressure gradient, no loss gun system. A comparison of predicted to measured muzzle velocities is made for a number of fielded and experimental guns; several hypothetical systems are also examined. The comparison of calculated muzzle velocities permits an assessment to be made of the importance of chemical reactivity throughout the ballistic cycle.

INTRODUCTION

The limiting case of the constant breech pressure (CBP) gun is often invoked to predict the maximum velocity or efficiency of a gun system [1-3]. Typically this calculation is done using a Lagrange pressure gradient and by casting propellant energetics, usually derived from thermochemical equilibrium calculations, in forms (mainly γ, impetus, and the covolume) compatible with the Noble-Abel equation of state. A nominal gas phase density (usually 0.2 g/cm^3) is assumed, from which effective energetics are calculated; traditionally these are taken as those of the equilibrium mixture of combustion gases for constant volume, adiabatic conditions. For the actual interior ballistic calculation, however, the resultant chemical composition determined for this arbitrary equilibrium state is considered to be "frozen"; that is, it is assumed to be chemically inert throughout the entire ballistic cycle. In this study, constant breech pressure gun calculations are performed with full equilibrium chemistry obtaining throughout the ballistic cycle. The calculations are performed using a standard chemical equilibrium code, BLAKE [4], without any further modifications. The three well-defined thermodynamic states that completely characterize the energetics of this gun system are identified. Thus, the processes delineating propellant performance (and the conditions at muzzle) are readily calculated using full, variable composition, equilibrium thermodynamics. Since the thermodynamic states are totally determined by the design parameters of the gun and by the limiting condition of infinitely fast chemistry (equilibrium), no arbitrary gas phase density or chamber condition needs to be assumed. This method, therefore, represents an "exact" calculation of the optimized constant breech pressure (before burnout), Lagrange pressure gradient, no loss gun system. A comparison of predicted to measured muzzle velocities is made for

a number of fielded and experimental guns; several hypothetical systems are also examined. The comparison of the muzzle velocities obtained by this exact method of calculating the constant breech pressure gun problem (reacting, exact energetics) to that of the traditional method (nonreacting, effective energetics) then permits an assessment to be made of the importance of variable chemistry in determining propellant efficiency [5] in gun systems.

IDEALIZED CBP GUN WITH VARIABLE THERMOCHEMISTRY

The method of calculation utilizes a thermodynamic state description of the ballistic cycle. There are several steps that need to be considered to understand the process, but only three states of the system need to be calculated. The characteristic features of this system are a constant pressure portion which lasts from the time the operating pressure is reached (shot start) to the time the solid propellant is entirely consumed (burns out); this is followed by the reversible isentropic expansion of the gases until the end of the tube is reached (muzzle condition). The co-ordinates of the gun are shown in Fig. 1.
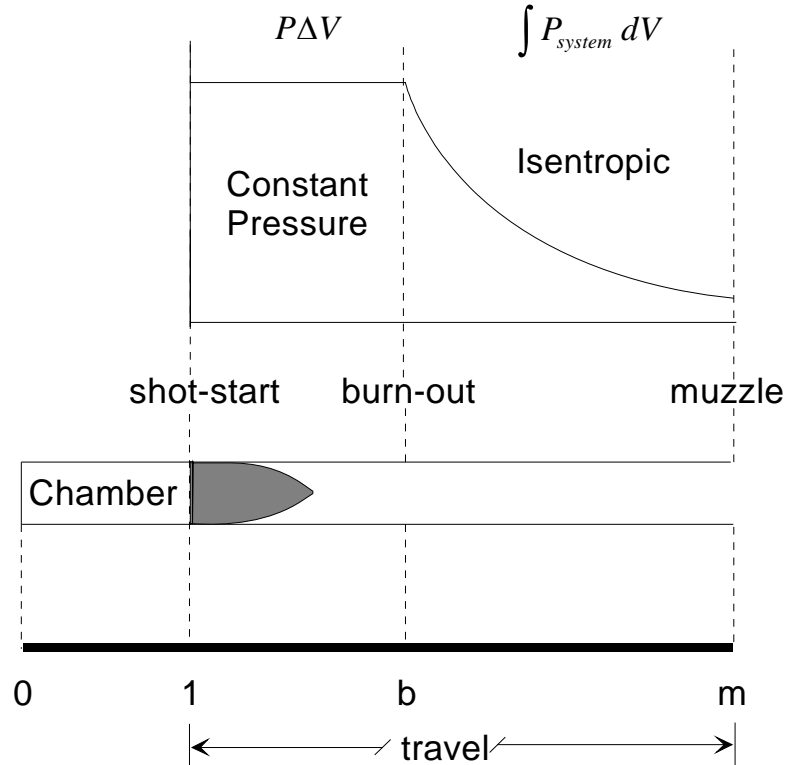

Figure 1 Coordinates for the constant breech pressure gun.

The Use of BLAKE

BLAKE will be used to perform the calculations, however, the method relies on basic thermodynamic principles and is not tied in any way to BLAKE itself. BLAKE is chosen because it allows for real gas effects and has the apparatus in place to calculate the designated states.

Description of the Problem

The process is adiabatic so for each step Q=0. The breech pressure, also called the chamber pressure, is given and is determined by known operating parameters (design parameters) for the gun. A Lagrange gradient is assumed. The method of Lagrange is often used and is dealt with elsewhere [6]. The use of the Lagrange gradient allows a partitioning to be made of the total energy, in the form of work, done by the system. The system here is the propellant, which hereafter, will be used to refer to the total matter, of any phase or composition, that comprised the original unburnt propellant; the system, however, does not include any bulk kinetic energy of the propellant.

Consequently, the internal energy of the system, U, includes the thermal and chemical energy of the system, but not any bulk kinetic energy, $KE_{Propellant}$. Strictly speaking, the total energy, E, of the system is

$$E_{system} = U + KE_{Propellant}.$$

Note that, in keeping with the Lagrange assumptions, the solid is considered to be uniformly dispersed throughout the system volume.

BLAKE will only calculate the internal energy, U. The relationships that follow from the choice of the Lagrange gradient assumption are used to partition the change in internal energy, ΔU, between the kinetic energy of the combustion gases and the projectile

$$\Delta U = KE_{Propellant} + KE_{projectile}.$$

Thus, the change in internal energy of the system results in work on the surroundings which manifests itself as kinetic energy (velocity) of the propellant and the projectile.

Method of Calculation

Only three states need to be calculated. Each of these states is now considered.

State 1 - Initial. For the initial state, the internal energy of the propellant must be calculated. The initial state of a propellant is usually at ambient conditions taken here to be P=1 atm and T=298.15 K. These are also the conditions for which the standard enthalpy of formation is tabulated. This is also the reference T and standard pressure for BLAKE's assigned energy scale, consequently, for condensed-phase propellants, $U \approx H = (\Delta H_f^o)_{298.15K}$ [7]. The internal energy of the initial state, U_0, can therefore be calculated from the tabulated $(\Delta H_f^o)_{298.15K}$, the proportions of the components, the chemical formulas, and atomic weights.

State 2 - Burnout. The energy of the state at burnout, U_b, is calculated from the internal energy of the propellant and the work done along the constant pressure path that is specified as a design parameter of the gun. Identification of this state is the key to performing the calculation. It is straightforward to write

$$U_b = U_0 - W,$$

where for the total work

$$m_c W = P(m_c V_{0b} - V_C)$$

and for the mass specific work

$$W = P(V_{0b} - V_{0C}),$$

where $V_{0C} = V_C /m_c$, V_C is the volume of the chamber, and m_c is the mass of the charge (the propellant).

Using the relationship

$$U_b = H_b - P V_{0b},$$

$$H_b - PV_{0b} = U_0 - PV_{0b} + PV_{0c},$$

$$H_b = U_0 + PV_{0c},$$

or

$$H_b = U_0 + P V_c/m_c.$$

Thus the thermodynamic state at burnout is fully specified by the operating pressure and the enthalpy at burnout as indicated, where U_0, the initial internal energy, P, the operating pressure, V_c, the chamber volume, and m_c, the charge mass, are all known design parameters.

State 3 - Muzzle. From the state at burnout, a reversible adiabatic expansion takes place to muzzle. For a reversible expansion $dS = \delta Q_{rev} / T$. Since the process is adiabatic, $\delta Q_{rev}=0$, and the expansion proceeds along a constant entropy path. This is easily calculated by BLAKE using the value of the entropy at burnout, holding it constant, and going from the specific volume at burn-out to the specific volume at muzzle which can be calculated from the design parameters; *i.e.*, at muzzle

$$V_m = V_{Total} / m_c,$$

where V_{Total} , the total volume, is the sum of the chamber and tube volume

$$V_{Total} = V_{chamber} + V_{tube}.$$

Gun Systems Analyzed

The systems studied in this work fall into three categories: actual fielded systems, experimental or research systems, and hypothetical.

Fielded Systems. The majority of systems in this category are the 249 guns and howitzers listed in the STAR report [8]. The range of the system parameters are:
1. nominal tube diameters of 40 mm, 105 mm, 120 mm, 152 mm, 155 mm, and 8 inch (205 mm)
2. travel, 1.4-6.9 m
3. chamber volume, 0.475-32 liter
4. charge mass, 0.09-22.5 kg
5. projectile mass, 0.9-90.7 kg
6. P_{max}, 31-528 MPa.
Charges consisted of propellants M1, M30A1, M6, M9, M30, JA2, M26E1, M17, M30A2, M31A1, and M2. Formulation for the calculations are from Freedman [9]. In addition to these systems, several guns treated in the CONPRESS report [3] are also calculated.

Experimental Systems. This category includes several hypervelocity gun firings [10, 11], including a High-Altitude Research Program (HARP) gun [12].

<u>Hypothetical Systems.</u> This category includes several systems using GAP/ADN and GAP/CL20 as propellant [13].

RESULTS AND DISCUSSION

Calculations were performed using the traditional method of calculating theCBP gun problem; the equations describing this problem, which does not allow reactive chemistry or temperature variation of the thermodynamic properties of the system, are well known [3]. Calculations were also performed using the method described in the previous section, utilizing the full thermochemical description of the ballistic cycle. These are respectively called ConP and ChemP. Results for the STAR report systems are summarized in Figs. 2 and 3. Fig. 2 is a plot of the ballistic ratio (BR)
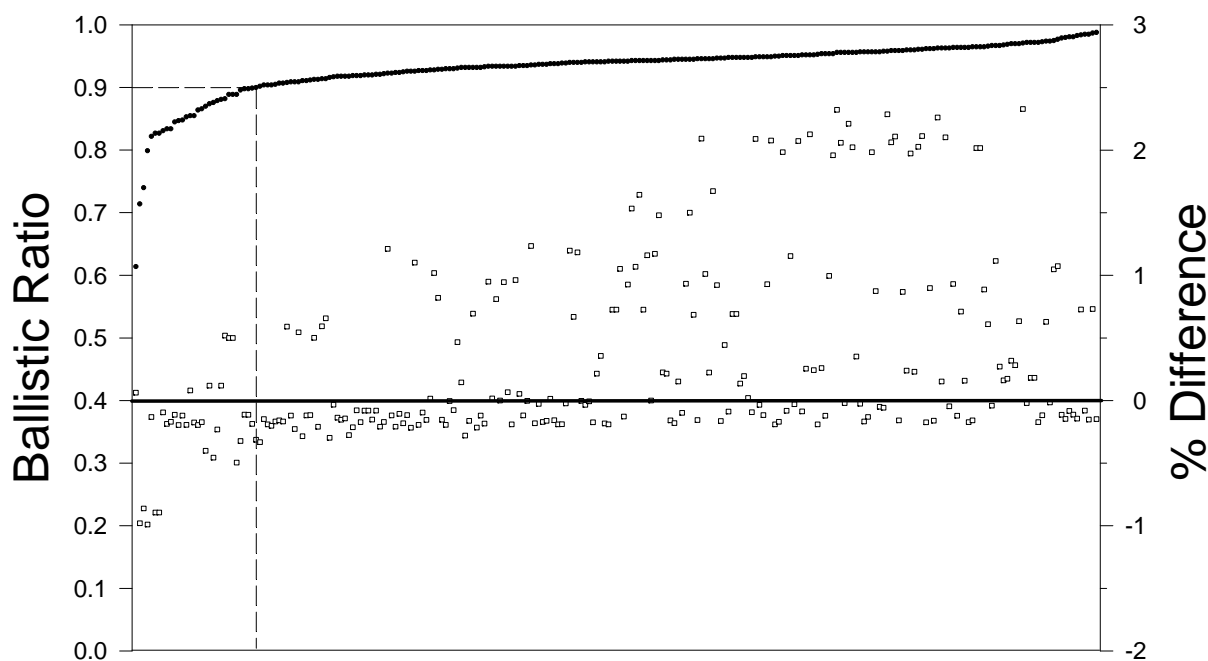

Figure 2 Ballistic Ratio and % Difference for the guns and Howitzers in the STAR Report. (●) Ballistic Ratio, (□) %Difference.

which is defined as the ratio of measured muzzle velocity to the calculated (ChemP) muzzle velocity. There is no significance to the x axis; each point is for one of the gun systems which are ordered according to the value of the ballistic ratio. Also plotted is the %Difference (%diff) between the two methods, defined arbitrarily as $(v_{ConP}-v_{ChemP})/v_{measured}\times100\%$. $v_{measured}$ is used here as an unbiased scaling factor. Because of this definition of %diff, and the fact that both calculated values are always higher than the measured velocity, negative values indicate instances where the ChemP velocity is the greater and, therefore, farther removed from the measured; positive values indicate instances where the ConP velocity is the greater and, therefore, farther removed from the measured. Since the actual gun is expected to have losses and exhibit less-than-ideal behavior, a calculated value that is

closer to the measured is not necessarily more accurate. However, the two methods do track the measured velocity differently, with ConP values differing from ChemP values by up to 2.5% when it is the greater of the two and, therefore, farther removed from the measured value. Conversely, ChemP differs by about 1% when it is greater. However, 31 guns have ballistic ratios lower than 0.9, a value that has been previously noted [1,3] as the lower limit for which actual systems can still be taken as approaching the CBP idealization. This may be used as a somewhat arbitrary, but reasonable, discriminator; the dashed lines in Fig. 2 are drawn for this value. The values to the left of the vertical dashed line can therefore be discounted, since they are examples of systems that do not approach the CBP idealization. If this is done then for instances where $v_{ChemP} > v_{ConP}$, the difference between the two is less than 0.4%; however, when $v_{ConP} > v_{ChemP}$, the difference can be almost 2.5%.

A question arises as to why 31 guns fall below the BR=0.9 value. Fig. 3 is a plot of the BR versus measured velocity (The lowest BR value may result from an incorrect charge mass in the STAR Report). Guns below the BR=0.9 discriminator are low velocity systems with measured muzzle velocities less than 550 m/s. A number of these are low zone charges for which, presumably, it was not necessary that the system be optimized; however, the higher velocities in this group are high zone (6 and 7) charges. Fig. 3 also shows many low velocity systems that have a high BR; the higher velocity guns (v > 1100 m/s) represent optimized systems for which the ballistic ratios are all greater than 0.95.

Figure 3 Ballistic Ratio (ChemP) for systems in the STAR Report.

Several systems are often cited [3] to illustrate the applicability of the CBP idealization to a variety of configurations. These have been recalculated here using the two methods, and are given in Table 1. Trends are similar to those of the systems in the STAR report.
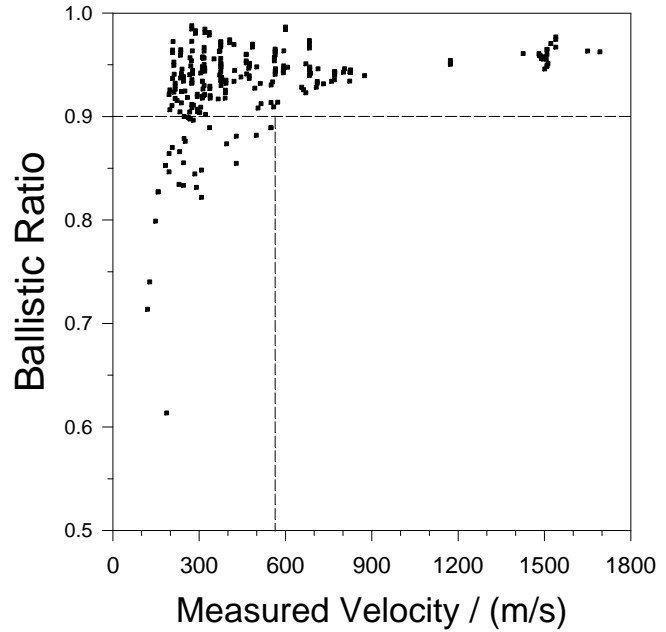
Gun	muzzle velocity / (m/s)			%diff	BR	propellant
	measured	ConP	ChemP			
IMI	1,620	1,784	1,743	2.6	0.93	M30
M68	1,486	1,575	1,544	2.1	0.96	M30
M256	1,650	1,712	1,678	2.0	0.98	JA2
XM25	1,739	1,796	1,765	1.7	0.99	JA2
Navy 5"/54	808	868	864	0.5	0.93	NACO
M198	826	884	871	1.5	0.93	M30A1

Table 1 CBP and measured velocities for typical gun systems.

Table 2 summarizes the results for a double-travel, 120-mm, hyper-velocity gun. For this experimental gun, the largest difference between velocities calculated using the two methods, 3.2%, corresponds to an actual velocity difference of 81 m/s. For all the entries in this table, $v_{ConP} > v_{ChemP}$. Another example in this category is a HARP gun [12]. This system had a BR≈1, with v_{ChemP} =2820 m/s, just 2 m/s more than the measured value.

Another regime considered was purely hypothetical systems and consisted of 120-mm, 132-mm, and 156-mm-diameter guns with high impetus (*ca*. 1,300 and 1,400 J/g) GAP-ADN-CL20 propellant [13]. Nominal results were obtained for this series of six configurations except for the longest travel (6.88 m) 156-mm-diameter gun for which the difference between the two methods was -1%.

SUMMARY & CONCLUSION

A simple yet exact, thermodynamic state specific method for calculating the Lagrange gradient, constant breech pressure, no loss gun, allowing full equilibrium thermo-chemistry throughout the ballistic cycle, is presented. As an exact

muzzle velocity / (m/s)			Δv / (m/s)	%diff	BR	Ref.
measured	ConP	ChemP				
2,057	2,265	2,241	24	1.2	0.92	
2,190	2,359	2,324	35	1.6	0.94	
2,237	2,399	2,358	41	1.8	0.95	10
2,279	2,436	2,390	46	2.0	0.95	
2,311	2,464	2,421	43	1.9	0.95	
2,455	2,562	2,492	70	2.9	0.99	10
2,499	2,602	2,521	81	3.2	0.99	
2,686	2,774	2,710	64	2.4	0.99	
2,678	2,775	2,711	64	2.4	0.99	
2,666	2,766	2,704	62	2.3	0.99	11
2,278	2,417	2,373	44	1.9	0.96	
2,272	2,422	2,377	44	2.0	0.96	
2,273	2,430	2,384	46	2.0	0.95	
2,584	2,728	2,664	64	2.5	0.97	
2,522	2,643	2,585	58	2.3	0.98	
2,480	2,647	2,589	58	2.3	0.96	11
2,284	2,419	2,369	50	2.2	0.96	
2,283	2,424	2,375	49	2.2	0.96	
2,595	2,663	2,630	33	1.3	0.99	
2,579	2,651	2,619	32	1.2	0.98	
2,586	2,653	2,621	32	1.2	0.99	11
2,291	2,384	2,356	28	1.2	0.97	
2,292	2,382	2,354	28	1.2	0.97	
2,300	2,385	2,357	28	1.2	0.98	

Table 2 Comparison of hypervelocity gun results. $\Delta v \equiv v_{ConP}\text{-}v_{ChemP}$; propellant, JA2.

calculation of this idealized gun, it represents a true limiting, maximum value for the muzzle velocity and available kinetic energy. Since it does not invoke an arbitrary choice of gas phase density to predict the system's energetics, as does the traditional method, it represents a self-consistent description of the idealized gun. This method typically predicts muzzle velocities that are lower than velocities calculated by traditional methods, which do not allow chemical reactions throughout the ballistic cycle, by up to 3.2% (81 m/s). In general, muzzle velocities calculated by the traditional approach, which uses "frozen," temperature invariant, effective thermochemistry estimated at 0.2 g/cm^3 density under adiabatic, constant volume conditions, are found to be very close to the exact solution for a wide variety of gun systems.

ACKNOWLEDGMENTS

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